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Fairfax Materials Research Inc.

5613 Marble Arch Way
Alexandria, Virginia 22310-4011

(703)-922-4579 Fax: (703)-922-6034

Feb. 28 1994

Dr. A. K. Vasudevan, code 1222
Office of Naval Research
800 N. Quincy Street
Arlington, VA 22217-5000

re: Contract #N00014-91-C-0067

Dear Dr. Vasudevan:

Please find attached one copy of the quarterly (December-February) technical report in accordance with the contract above.

Work during this last quarter has centered on cyclic deformation of high-temperature materials.

Yours sincerely

Dr. M.S. Duesbery
Vice-President
Fairfax Materials Research, Inc.

cc: ACO
NRL
DTIC (2)

Computer Modelling of Cyclic Deformation of High-Temperature Materials

TECHNICAL PROGRESS REPORT

Dr. M.S. Duesbery
Principal Investigator

Dr. N.P. Louat
Senior Scientist

Fairfax Materials Research, Inc.

5613 Marble Arch Way
Alexandria, VA 22310-4011

February 28, 1993

Period of performance
December 1, 1993 through February 28, 1994

I. Introduction and Program Objective

Current methods of lifetime assessment leave much to be desired. Typically, the expected life of a full-scale component exposed to a complex environment is based upon empirical interpretations of measurements performed on microscopic samples in controlled laboratory conditions. Extrapolation to the service component is accomplished by scaling laws which, if used at all, are empirical; little or no attention is paid to synergistic interactions between the different components of the real environment. With the increasingly hostile conditions which must be faced in modern aerospace applications, improvement in lifetime estimation is mandated by both cost and safety considerations.

This program aims at improving current methods of lifetime assessment by building in the characteristics of the micro-mechanisms known to be responsible for damage and failure. The broad approach entails the integration and, where necessary, augmentation of the micro-scale research results currently available in the literature into a macro-scale model with predictive capability.

In more detail, the program will develop a set of hierarchically structured models at different length scales, from atomic to macroscopic, at each level taking as parametric input the results of the model at the next smaller scale. In this way the known microscopic properties can be transported by systematic procedures to the unknown macro-scale region. It may not be possible to eliminate empiricism completely, because some of the quantities involved cannot yet be estimated to the required degree of precision. In this case the aim will be at least to eliminate functional empiricism. Restriction of empiricism to the choice of parameters to be input to known functional forms permits some confidence in extrapolation procedures and has the advantage that the models can readily be updated as better estimates of the parameters become available.

II. Program Organization

The program has been organized into specific tasks and subtasks as follows.

Task 100. Lifetimes of metallic dispersed-phase composites

Most service materials fall into the category of dispersion-hardened metallic composites. This task will consider the problem of dispersion hardened materials in general, but with two specific materials, NiAl and $MoSi_2/SiC$ in mind.

Task 110. Identification and modelling of micromechanisms

The purpose of this task is to determine what micromechanisms are operative in the high-temperature deformation of dispersion-hardened materials. In the general case this will be done by a literature search. For specific materials, the micromechanisms will be determined from the experimental program at NRL. Once identified, each of these micromechanisms will be modelled, in order to determine what are the critical parameters which determine its effect on plastic flow and values for these parameters. Also to be determined is whether the modelled critical values are dependent on quantities which must be obtained from a smaller scale model.

Task 111. Equiaxed dispersoids

This task will consider dispersions of the type encountered in NiAl-like materials. That is, the dispersoids are considered to be small compared to the grain size. The term 'equiaxed' is used because the particles are roughly of the same size in all three dimensions. However, this is not a requirement for this task. Rather, it is necessary that the particles not be too large in the dimension normal to the slip plane, so that they can be surmounted with relative ease by cross-slip and/or climb without the generation of appreciable back-stress.

Task 112. Anisotropic dispersoids

This task covers the case of dispersoids which are elongated in the direction normal to the slip plane. An example is SiC fibers in $MoSi_2$. In this case, plastic flow around the dispersoids takes place by a combination of glide and climb, but is a protracted process during which large stresses acting in opposition to the applied load are developed.

Task 113. Grain boundary effects

This task will examine the role of grain boundary processes in high-temperature deformation.

Task 120. Macroscopic stochastic model for creep

In real materials it is likely that more than one mechanism will be operative, either in parallel or in series. The information gained in task 110 is not sufficient to describe this situation. Once the critical parameters for individual mechanisms have been determined, it is necessary to combine them in a macroscale stochastic model. This will be done by determining critical stresses and activation enthalpies as a function of local geometry and using these values in a finite-temperature simulation of creep through a random array of dispersoids. Careful attention must be paid to possible interactions between mechanisms.

Task 130. Extension to cyclic deformation

The final step in task 100 is to extend the results to the case of cyclic deformation. Irreversibility is an intrinsic feature of the model in task 120. However, it is likely that other, as yet unrecognized, characteristics of cycled deformation will have to be considered.

Task 200. Lifetimes of piezoelectric ferroelectrics

Failure in cyclic loading of sensors and actuators formed from lead zirconate titanate (PZT) is a continuing problem. PZT is a ceramic and therefore differs from the materials considered in task 100 in that plastic deformation is not involved. This task will examine, modelling as necessary, the operation of PZT devices, in order to determine the factors governing lifetime limitation.

Task 300. Reporting

Running concurrently with tasks 100 and 200, this task will inform the Navy Program Manager and Contracting Officer of the technical and fiscal status of the program through R&D status reports.

III. Technical Progress

Task 100. Lifetimes of metallic dispersed-phase composites

Task 110. Identification and modelling of micromechanisms

Cyclic Deformation

We are concerned to examine the effects on ΔK consequent on a failure to achieve complete crack closure upon removal of an applied load. Such a failure has been severally attributed to two causes: (1) the presence of a mismatching surface asperity or protrusion and (2) the effects of plastic deformation. The analysis given here deals with these in turn.

The Effects of Asperities

In the interests of mathematical simplicity and without prejudice to the conclusions, we depart from normal experimental conditions and consider a two dimensional crack which lies in the interval $|x| \leq a$ of the plane $y = 0$ of a body subjected to an externally applied, time dependent tensile stress σ, which varies from zero to σ_{yy}. In these circumstances we have:

$$\Delta K = \sigma_{yy}\, a^{1/2}/2^{1/2}.$$

At a stress σ prior to any encounter with asperities the crack surfaces at a distance $|x| = c$ from the center of the crack will have suffered an elastic displacement of magnitude:

$$\Delta = \sigma \frac{\lambda}{\pi A}\sqrt{(a^2-c^2)}$$

where $A = \mu\lambda/2\pi(1-\nu)$, μ is the shear modulus, ν is Poisson's ratio and λ is the magnitude of the Burgers vector of a unit dislocation. In the interests of mathematical simplicity we suppose symmetry about the crack center so that asperities occur in pairs of height δ, that they both make contact when the stress is τ at $|x| = c$ and impede crack closure at all stresses less than τ. We can, at this stage, suppose either that the asperities are rigid so that the displacement, δu, at $|x| = c$ remains equal to δ as the applied stress is reduced below the value τ or alternatively that δu declines to some equilibrium value as the asperities and their environs in the surfaces deform either elastically or plastically or both under the compressive loads developed in them. The latter approach is the more realistic and will be that finally adopted here. However, the treatment necessary when the asperities are considered to be rigid is much more general. Accordingly, we shall for the sake of completeness take the general treatment through to the stage where specification of deformation in the asperities becomes necessary.

We divide the crack into three segments: $|x| \leq c$, $c \leq |x| \leq b$, $b \leq x \leq a$; $c \approx b$. We then follow the well known technique first introduced by Leibfried [1] and independently by Head and Louat [2] which employs the concept of dislocation continua to describe the situation in each of these ranges in terms of an equation of equilibrium.

We have for the distribution f(x) of dislocation over the length of a crack:

$$A\int_D f(x)\frac{dx}{x-t} = \sigma(t)$$

where integration is over the union of intervals, D, in which dislocation occurs and $\sigma(t)$ is the stress applied at the point $0 \le t \le a$. . The solutions of such equations have been given by Muskhelishvili (3) and by Louat (4). In the present case which involves three intervals, the solution is of the form:

$$f(x) = \frac{-\sigma}{\pi^2 A\sqrt{(x^2-c^2)(b^2-x^2)(a^2-x^2)}}\int_D \sqrt{(t^2-c^2)(b^2-t^2)(a^2-t^2)}\frac{dt}{t-x}$$

$$+\frac{Q}{\sqrt{(x^2-c^2)(b^2-x^2)(a^2-x^2)}}$$

where Q is an arbitrary polynomial of the second degree. From symmetry we choose Q to be of the form S^2x , where S is a parameter such that the number of dislocations in the interval $b \le |x| \le a$ is, for stresses less than τ, equal to δ_c/λ. To satisfy this requirement we set

$$S^2 = \sigma d^2 + e$$

so that:

$$f(x) = \frac{x}{\sqrt{(a^2-x^2)(b^2-x^2)(X^2-c^2)}}\left(\frac{\sigma}{\pi A}(-x^2+d^2)+e\right)$$

Here we discern two contributions to the whole distribution, only one of which is dependent on stress. This stress sensitive distribution (in σ) vanishes at $x = d$ which is chosen so that the total associated displaacement in the range $b \le |x| \le a$ is zero. Thus, integrating that part of the distribution which depends on σ we require that:

$$(c^2-d^2)\frac{K(k)}{\sqrt{(a^2-c^2)}}+\sqrt{(a^2-c^2)}E(k)=0,$$

which when rearranged becomes:

$$d^2=c^2+(a^2-c^2)\frac{E(k)}{K(k)}. \qquad (1)$$

Here K(k) and E(k) are, respectively, complete elliptic integrals of the first and second kinds; the quantity k is given by:

$$k = \{(a^2 - b^2)/(a^2 - c^2)\}^{1/2}.$$

In the other distribution, which is independent of stress, the quantity, e, is such that the total number of dislocations in the same interval is equal to a number δ / λ. Thus, we require that:

$$\delta = \frac{\tau \lambda \sqrt{a^2-c^2}}{\pi A} = \lambda \int_D \frac{e\, dx}{\sqrt{(a^2-x^2)b^2-x^2)(x^2-c^2)}} = \frac{2e\lambda K(k)}{\sqrt{a^2-c^2)}};$$

$$e = \frac{\tau(a^2-c^2)}{2\pi A K(k)}. \qquad (2)$$

We are here concerned, in particular, with conditions which apply when the load has been removed so that σ is zero. In these circumstances and for the rigid asperity the distribution function becomes:

$$f(x) = \frac{ex}{\sqrt{a^2-x^2)(b^2-x^2)(x^2-c^2)}}.$$

The stress intensity is then readily evaluated by calculating the stresses at a point t at the tip of the crack:

$$A \int_D \frac{f(x)dx}{x-t} = \pi A f(t).$$

In the case of deformable asperities, the value of e must be such that the stress developed therein has some characteristic value τ_c which is associated with a surface displacement δ_c. In small plastically deformable materials (e.g. metallic whiskers) this stress is of order:

$$\frac{\mu b}{D}$$

where D is the least linear dimension of the cross section of the material; here D = b - c. In the cases where the asperity itself is not deformable it must be considered to be supported at its ends by on material which is deformable. The stresses in the deformable regions adjacent to the areas of impingement will be of the same order as that in the asperity itself. We conclude, therefore, that we can achieve an adequate representation by supposing that

$$\tau_c = \frac{\mu b}{D} \equiv \frac{\mu b_0}{b-c}. \qquad (2)$$

where b_0 is the Burgers vector of a lattice dislocation.

The stresses in the asperities are readily evaluated. The stress $\sigma(t)$ at a point t, which lies in an asperity, due to the elastic displacements of the surfaces of the crack is given by:

$$\sigma(t) = A \int_D \frac{f(x)dx}{x-t}.$$

The mean value of this stress over the length, (b-c), of the asperity is

$$\frac{-\pi AeK(p)}{(b-c)\sqrt{a^2-c^2}}; \qquad (3)$$

$$p = \sqrt{\frac{b^2-c^2}{a^2-c^2}}.$$

Equating (2) and (3) we find that

$$e = \frac{2(1-\nu)b_0\sqrt{a^2-c^2}}{\lambda K(p)}.$$

We are now in a position to evaluate δ_c. We have

$$\delta_c = \int_b^a f(x)dx = \frac{2e\lambda K(k)}{\sqrt{a^2-c^2}}.$$

Thence, substituting for e we find

$$\frac{\delta_c}{b_0} = \frac{4(1-\nu)K(k)}{K(p)}$$

For the primary range of interest in which $(b-c)/(a-c) << 1$ we determine that K(k) lies in the range $\pi/2$ to 10 while $K(p) \approx \pi/2$. Accordingly:

$$\sim 3 \leq \frac{\delta_c}{b_o} \leq \sim 20.$$

In the case of the other possible range in which a-b becomes very small K(p) exceeds K(k) indicating improbable situations in which $\delta_c/b_0 < 1$.

The remnant value of ΔK, that consequent on the crack being held open at a points distant c from its centre by asperities of height δ_c may be determined by calculating the stress at the tip of the crack. On substituting for e the stress at any point, t, outside the crack, is easily seen to be:

$$Ae\int_D \frac{xdx}{\sqrt{(x^2-a^2)(x^2-b^2)(x^2-c^2)(x-t)}}$$

$$= \frac{\mu b\ \sqrt{a^2-c^2}\ t}{2K(p)\sqrt{(t^2-a^2)(t^2-b^2)(t^2-c^2)}}.$$

When t = a + Δ, Δ << a, this becomes

$$\sim \frac{\mu b\ a\ \sqrt{a^2-c^2}}{2K(p)\sqrt{(2a\Delta)(a^2-b^2)(a^2-c^2)}} = \frac{K}{\Delta^{1/2}}.$$

Therein,

$$K = \frac{\mu b_o a}{2\sqrt{2}K(p)\sqrt{a^2-c^2)}}$$

$$\sim \frac{\mu b_0}{4K(p)\sqrt{a(a-c)}}.$$

Taking appropriate values: a = 1 cm.; b = $3X10_{-8}$ cms.; a-c ≥ $300X10^{-8}$ cms. and; K(p) = π/2, we have

$$K \leq \frac{\mu}{6\ X\ 10^5}.$$

This represents a value for ΔK which is much smaller than those employed in practice. We conclude, therefore, that the existence of misclosure from the presence of asperities can give only a minimal change on the effective value of the applied ΔK.

The final matter of consideration here is the possibility, first suggested by Elber [19], of premature crack closure consequent on the effects of residual stresses due to plastic deformation in the neighbourhood of the crack tip. We will proceed to show on the basis of dislocation theory that the associated crack surface displacements are too small to provide such closure. In so doing we shall run counter to the results of analyses based on plasticity theory which have indicated contrary results. An examination of the this work indicates that since our treatment does not involve a model the probable source of the discrepancy lies in the assumptions involved in the models employed by the plasticians.

To proceed, we note that plastic deformation is necessarily achieved as the result of the formation and movement of dislocations. We recognize also, that the displacement engendered by a dispersion of dislocations is representable as the result of a linear superposition of the displacements due to the individual dislocations. In the first instance we particularize to plain strain and see that the dislocations in the neighbourhood of a crack tip have been formed either by the symmetrical operation of sources in the material or by asymmetrical emission from (or absorption by) the crack. Taking the crack to lie in a plane y = constant, emitted dislocations may be regarded as having components b_x and b_y in the x- and y- directions. This asymmetrical formation is associated with a displacement (b_y) of the crack surfaces. We recognize, that besides these displacements, each dislocation may, in the first instance, be regarded as causing elastic displacements of the surfaces which are just those of a dislocation in an infinite medium. Referred to the position of a dislocation, the important y-component of displacements due to the y-component of an edge dislocation can be written:

$$u_y = -\frac{b_y}{4\pi(1-\nu)}\frac{xy}{(x^2+y^2)} + 2\frac{b_y}{\pi}\arctan(x/y)$$

Again, the y-component of displacement of a dislocation with Burgers vector in the x-direction is:

$$U_y = (1-2\nu)\frac{b_x}{8\pi(1-\nu)}\ln\frac{(x^2+y^2)}{b^2} - b_x\frac{y^2}{4\pi(1-\nu)(x^2+y^2)}.$$

Neither component of this displacement is significant here; the logarithmic term diverges but gives a value, comparable with the magnitude of the Burgers vector, only at distances along the crack surface conveniently measured in miles.

Surface displacements are also developed in order that the surface be stress free. These displacements can be found through the use of the approach [Louat, 1963] in which the derivative of such displacements are recognized as being representable as distributions of dislocations. Thus, we take as a condition for equilibrium:

$$\int_0^\infty f(x)\frac{dx}{(x-t)} = \sigma(t)$$

The solution of this equation is given by

$$f(x) = -\frac{1}{\pi^2 A\sqrt{x}}\int_0^\infty \sqrt{t}\,\sigma(t)\frac{dt}{(t-x)}.$$

Now, in an infinite solid, an asymmetrically produced dislocation which has a Burgers vector b_y

and which is located at the point (0,y), referred to the crack tip , produces a stress, σ_{yy} , at the positions of the line of the crack surfaces of amount:

$$\frac{\mu b_y\, y(3x^2-y^2)}{2\pi(1-\nu)(x^2+y^2)^2}$$

The displacement at a point x_0 is then given by:

$$\int_0^{x_0} f(x)dx = \frac{b}{\pi^2}\int_0^{x_0}\frac{dx}{\sqrt{x}}\int_0^{\infty} t^{3/2}\left(2-\frac{d}{dy}\right)\frac{y}{(Y^2+t^2)}\frac{dt}{(t-x)}$$

$$= \frac{b}{4\pi}\left(2-\frac{d}{dy}\right)\ln\frac{x_0^2+\sqrt{2}x_0y+y^2}{x_o^2-\sqrt{2}x_0y+y^2}$$

This displacement is additive to, but less than and of the opposite sign to that of the rigid displacement involved in the formation of the dislocation. To illustrate the magnitudes involved, we note that when x_0 = y and $u_y \approx b_y/2$, this first, and dominant term, has a maximum of magnitude .28 b_y. It is zero when x $=\infty$.

Turning to the effects consequent on the presence of stresses σ_{yy} associated with the x-components of the Burger vectors of dislocations produced asymmetrically, we find in a similar fashion, displacements which have negative sign, a maximum of $-b_x/\sqrt{2}\pi$, again at x_0 = y, and which vanish at $x_0 = \infty$.

In summary we discern that, besides the surface displacements of dislocation formation there is a total of five other elastic contributions to the surface displacements. These are: the (three) appropriate infinite-solid-displacements (in the y-direction) due the two dislocation components, b_x and b_y and the (two) displacements which arise as a consequence of the normal stresses acting on the crack surfaces. Individual contributions are variable in sign and in total are seen by numerical evaluation to conform approximately at large distances from the crack tip to the major contribution, namely to that which arises in a infinite solid due to the y-component of the Burgers vector,namely:

$$2\frac{b}{\pi}\arctan(x/y)$$

Whence we see that closure is only just achieved under zero applied stress and at x $=\infty$.

Finally, we have to examine the effects of the remaining dislocations those produced in dipole pairs from the operation of symmetrical sources. Since the displacements due individuals of a dipole pair are of essentially of opposite sign, there are two effects, one towards crack closure the other favouring crack opening. Because of the constraints imposed by plastic deformation on the geometric disposition of the dipoles, the nett effect of individual pairs is apt to favour crack opening. Again, since their separations are generally less than the size of the plastic zone, dipolar effects on the surface displacements can be significant only at distances from the crack tip which are comparable with the size of the plastic zone. That is, at distances at which the effects of the asymmetrically produced dislocations are small.

We conclude, at least in the case of plain strain, that the displacements of the crack surfaces developed from plastic deformation at crack tips are incapable of causing closure under non-vanishing applied loads.

We now pass to a consideration of closure under plane stress conditions. We suppose that crack propagation has resulted in the appearance of a lip and, taking the most restrictive possible case, that this lip makes contact over the whole length of the crack when the applied load is removed. Proceeding as before we take the equilibrium dislocation function to be that appropriate for a uniform loading, σ_r over the whole length of the crack:

$$F(x) = \frac{\sigma_r}{\pi A\sqrt{a^2-x^2}},$$

so that the total displacement of crack surfaces is:

$$\int_0^a F(x)dx = \frac{\sigma_r a\lambda}{\pi A}.$$

Now, the stress σ_r is supposed to be applied uniformly over the crack surfaces, area: 2aH where H is the thickness of the plate. But the area available is only that provided by the lip thickness h : 4ha. This is fraction 2h/H of the plate area. The mean effective stress, σ_e, is:

$$\sigma_e = \frac{2\sigma_r h}{H}.$$

Taking reasonable values, h = 1μ and H = 1mm. we have

$$\sigma_e = \frac{\sigma_r}{500}.$$

If we suppose in conformity with our approach in dealing with asperities that

$$\sigma_m = \frac{\mu b}{h} \sim 3X\ 10^{-4}\mu,$$

we find that

$$\sigma_e = 6X\ 10^{-7}\ \mu.$$

This estimate could be increased if it were felt that the value adopted for μ_r is too small. Thus, we might take σ_r to be a few times the flow stress of the material in which case σ_c would a few hundredths of σ_r. This would still represent a value much smaller than the stresses normally applied to achieve fatigue. Even so such an increase can be expected to more than compensated for by the correction of the assumption that the plastic zone runs the full length of crack. The effect of this sort of misclose is thus seen to be of little moment.

Conclusions

We have seen that misclosure of a fatigue crack can have little effect on the effective value of ΔK. This has been found to be in both the case of asperites on the crack surface or and for that of the lips formed when fatigue occurs in a plate so thin that plane stress conditions have significant effects.

Again, we have found that plastic deformation in plane strain is incapable of providing crack closure at any fraction of the peak applied stress.

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